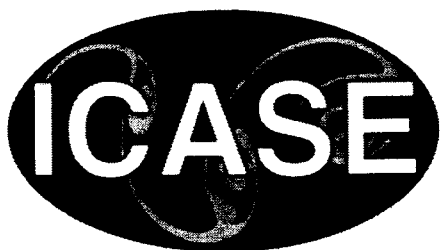


NASA/CR-2002-211756
ICASE Interim Report No. 42



Optimization of Designs for Nanotube-based Scanning Probes

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July 2002

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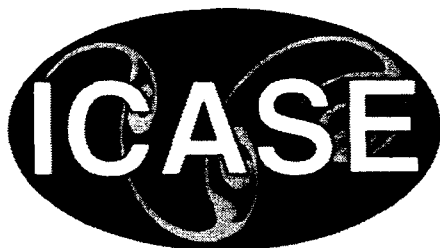
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Operated by Universities Space Research Association



Prepared for Langley Research Center
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OPTIMIZATION OF DESIGNS FOR NANOTUBE-BASED SCANNING PROBES

V. M. HARIK¹ AND T. S. GATES²

Abstract. Optimization of designs for nanotube-based scanning probes, which may be used for high-resolution characterization of nanostructured materials, is examined. Continuum models to analyze the nanotube deformations are proposed to help guide selection of the optimum probe. The limitations on the use of these models that must be accounted for before applying to any design problem are presented. These limitations stem from the underlying assumptions and the expected range of nanotube loading, end conditions, and geometry. Once the limitations are accounted for, the key model parameters along with the appropriate classification of nanotube structures may serve as a basis for the design optimization of nanotube-based probe tips.

Key words. carbon nanotubes, atomic force microscope, scanning probes, optimization

Subject classification. Computational Materials Science

1. Introduction. New types of nanostructured materials, such as carbon nanotubes, are being developed for a wide variety of applications. One of the principle difficulties associated with using nanostructured materials is the lack of precise imaging of the atomic structure. In recent years, scanning probe microscopy has matured dramatically and holds great promise for imaging and manipulation of nanostructures. Perhaps the most promising type of scanning probes for the characterization of nanostructured materials is the atomic force microscope (AFM) [1]. It is used for imaging and surface characterization *via* contact deformation or vibration measurements.

The probe section of the AFM typically relies on a sharp silicon tip attached to a thin cantilever beam [1]. As the tip approaches the material surface, it can reach a point that atomic forces can be detected and resolved by changes in the tip vibration frequency. That is, the forces acting on the tip and associated displacement can be measured by the AFM and used to establish relative position and arrangement of the atomic structure. The typical silicon-based tip is useful for many imaging needs; however, the dimensions of this tip are still considered large in comparison to nano-scale features of materials and may result in the loss of nano-scale image quality. The search for increasing the resolution of AFM has led to the use of single wall carbon nanotubes (SWNT) that are attached to the AFM tip [2, 3] thereby effectively decreasing the tip size (Fig. 1).

To realize highly accurate, quantitative images from the SWNT based probes, the static and dynamic behavior of the nanotube (NT) must be established analytically and verified experimentally. It is well known that NTs are cylindrical macromolecules composed of carbon atoms in a periodic hexagonal arrangement. These carbon NTs possess extraordinary physical properties [2-8] including high stiffness, strength, and electrical and thermal conductivities. Carbon NTs are often found with high aspect ratios [2-4] that make them ideal for the scanning probe-tip applications [5, 7]. In contrast to the conventional silicon scanning probes, NT's strength and structural resilience makes them wear-resistant and insensitive to frequent buckling and bending deformations.

In order to analyze this buckling, bending, and general mechanical behavior, SWNTs have been

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modeled using both molecular dynamics and continuum mechanics [2-5, 8-10]. However, because most molecular dynamics models are limited in size (millions of atoms) and time (pico seconds), it is desirable to firmly establish the ranges of applicability of continuum mechanics models that could be used to accurately describe the deformation of a SWNT in an AFM probe tip application [4]. These models could then be used in parametric studies to choose the best or optimum size NT for any potential imaging task.

Therefore, it is the intent of this paper to review several typical continuum models for thin shells and beams and determine their usefulness in describing SWNT deformation under a range of loading conditions representative of AFM probe tips. Many of the fundamental concepts of these models and their relationship to nanotubes are provided in references [4, 9, 10] and will be expanded upon in this brief report. These models can be utilized to provide a set of design curves that address loading conditions, end constraints, and NT geometries [4, 9]. These curves may then be used by the experimental or microscopy experts to select the optimum nanotube-based AFM probe tip.

As a key part of this brief review of NT-based probes, several important nanomechanical issues related to probe design are considered. This list of issues includes 1) ability of continuum models to describe deformation of molecular lattice structures, 2) effects of the NT structure on its deformation modes, 3) buckling of NT probes, 4) the role of NT end conditions and the load introduction, and 5) the effect of structural imperfections in NT response and, hence, on the accuracy of measurements.

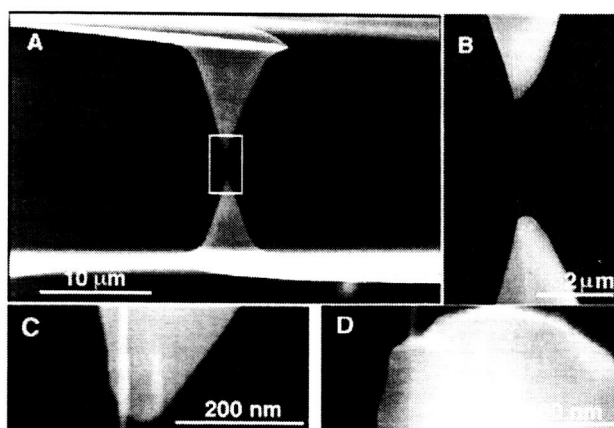


FIG. 1. Images of the prismatic silicon tips of the atomic force microscope (AFM) - AFM cantilever beams (A) and a nanotube attached to the silicon tips (B, C, D). Courtesy of Professor Rodney Ruoff (Northwestern University).

2. Design Considerations. Optimization of the NT-based scanning probes for structural response involves trade-offs between resolution and range. For example, the diameter of a NT probe tip influences its imaging resolution, thus a smaller diameter probe is desirable [7]. Likewise, the use of a NT tip of sufficient length increases the possible range required to image rough surfaces that involve steep asperities and deep openings. However, the resulting high aspect ratios of such long, thin NTs lead to unwanted flexibility of a NT tip that in turn reduces its scanning resolution. These types of trade-offs between resolution and range will be examined.

To analyze this type of nanomechanical problem, one needs to first consider typical loads (e.g., axial and off-axis) and the corresponding deformation modes. The loads can usually be related to the application such as lateral probe vibration (i.e., axial bending deformation), tapping mode (i.e., axial compressive loads) and translation-scanning mode (i.e., bending, radial and off-axis loads and friction forces) [1, 7].

Another consideration is the end conditions where the NT is attached to the base silicon tip. The flexibility of this attachment and the stiffness of the base silicon material will play a role in determining overall probe behavior.

The geometry of the NT (Fig. 2) also plays a significant role in determining overall behavior of the tip. As given by Table 1, current processing technologies produce nanotubes with wide variations in nanotube length (L_{NT}) and diameter (d_{NT}) [4]. In the NT structure, the distance of approximately 0.14 nm separates the adjacent carbon atoms, which is the length of the carbon-carbon covalent bond. A NT consists of many hexagonal carbon rings that have a width or side length (a) of 0.246 nm. Different arrangements of carbon rings determine the chirality and result in distinct NT geometries so that the diameter of a carbon NT is constrained by the number of carbon rings that fits into a NT circumference. For an end-loaded NT, the load transfer occurs through the highly directional covalent bonds [4]. The periodic hexagonal cell is the smallest periodic element in the NT lattice and its width can be identified as the characteristic dimension associated with the local NT structure. Due to the non-continuum aspects of NTs, the effective NT thickness, (h_{NT}) can only be estimated.

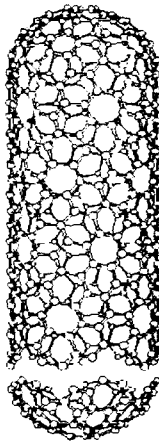


FIG. 2. Typical atomic structure of an end-capped, single walled carbon nanotube (after [11]).

Examination of the geometry of the NT leads to structure-property relationships and how these relationships may affect the mechanical behavior [4, 9]. For example, NTs of small radii have high transverse stiffness due to their tight structure, significant curvature and highly pre-strained covalent bonds. Such NTs behave like beams with the beam-type axial buckling mode. For a NT beam, the normalized radius is $R_{NT}/a \gg 1$. Under axial compression NTs with high aspect ratios behave like beams. The length-to-radius restriction $L_{NT}/R_{NT} \gg 1$ can be used to define these high aspect ratio NTs [9].

A large diameter NT has lower curvature and the covalent bonds are in a form that can be more closely approximated to a plain sheet of carbon atoms. Such NTs behave like thin shells and under axial loading may buckle with multiple wave patterns. A NT with thickness-to-radius ratio restriction $h_{NT}/R_{NT} < 1/20$ can be approximately modeled as a thin continuum shell [9].

In summary, we can group NTs into four general classes based on geometry; that is, thin NT shells, thick NT shells, high aspect ratio NTs, and thin beam-like NTs [4, 9]. This classification of NTs separates NT structures into groups that have similar global structural behavior, overall material properties, and deformation modes.

TABLE I
Geometric parameters of carbon NTs

Parameters	Range of Values
Width of a carbon ring,	0.246 nm
Diameter, d_{NT}	0.4 – 15 nm
Length, L_{NT}	1 nm – 10 μ m
Effective thickness, h_N	0.066 – 0.34 nm

3. An Example of the Analysis Method. For a nanotube probe, to prevent buckling and collapse leading to a loss of load carrying capability, the strain level at which nanotube buckling occurs should be determined. For NT shells, a linear shell buckling analysis can be carried out with a modification of the classical formula for continuum shells [8, 9]. However, the range of NT structural parameters should be properly limited before such a model is used. First, the proposed homogenization criteria ($L_{NT}/a > 10$), dictates a minimum length NT [4, 10]. This length criterion ensures unique averaging of NT material properties. Second, the range of values for NT radius depends on the choice of thin or thick NT shells [4]. That is, the buckling strain of the thin NT shells can be approximated by the following modified formula

$$(1) \quad \epsilon_{cr} = \frac{1}{\sqrt{3(1-\nu^2)}} \frac{h_{NT}}{R_{NT}},$$

only when the inequality $h_{NT}/R_{NT} < 1/20$ is satisfied and NTs have moderate aspect ratios. Here, ν is the Poisson's ratio. The approximate nature of this equation is recognized to be due to the assumption of material linearity and the sensitivity of shell buckling to small variations in thickness, cylindrical geometry and other nonlinear geometric effects [9].

For the class of NTs with high aspect ratio, ($L_{NT}/R_{NT} > 10$), the critical axial strain is proportional to the NT end-displacement and depends on the NT half-perimeter, R_{NT} , normalized by the NT length, L_{NT} :

$$(2) \quad \epsilon_{cr} = \frac{1}{2} \frac{R_{NT}}{L_{NT}} \sqrt{\frac{L_{cr}}{L_{NT0}}}$$

where L_{cr} is the critical end-displacement, L_{NT0} is the undeformed position, and $L = L_{NT0} - L_{NT}$. It should be noted that the moment of inertia, ($I = R^3 h$), the area, ($A = 2 R h$), Young's modulus, and the mechanical stress are not explicitly used in Eq. (2).

End conditions may play a role in modeling deformation. For example, the factor "1/2" in Eq. (2) can change according to the end conditions. In the example described here, the NT ends are simply supported. For the fixed ends, the critical strain is 4 times larger.

These analysis examples illustrate the utility and limitations of the continuum-based beam and shell models as applied to nanotubes. It would be expected that the continuum models could be used to perform initial design and selection (optimization) of the nanotube-based probes. This information would

then be carried forward to higher fidelity design and analysis including the use of molecular dynamics and molecular mechanics.

4. Summary: Optimization of Nanotube-based Probes. Design optimization of NT-based scanning probes for the AFM must account for nanomechanical loading conditions, end conditions, and NT geometry. There exist several continuum models that can provide quantitative estimates of NT deformation. However, the selection of the appropriate continuum model must be guided by a close examination of the assumptions and limitations imposed by the modeling method. With the appropriate model in hand, parametric studies can be conducted to establish the sensitivity of each model. These sensitivity studies can then be used to potentially select the optimum or best type of NT probe.

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE July 2002	3. REPORT TYPE AND DATES COVERED Contractor Report		
4. TITLE AND SUBTITLE OPTIMIZATION OF DESIGNS FOR NANOTUBE-BASED SCANNING PROBES		5. FUNDING NUMBERS C NAS1-97046 WU 505-90-52-01		
6. AUTHOR(S) V.M. Harik and T.S. Gates				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) ICASE Mail Stop 132C NASA Langley Research Center Hampton, VA 23681-2199		8. PERFORMING ORGANIZATION REPORT NUMBER ICASE Interim Report No. 42		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Langley Research Center Hampton, VA 23681-2199		10. SPONSORING/MONITORING AGENCY REPORT NUMBER NASA/CR-2002-211756 ICASE Interim Report No. 42		
11. SUPPLEMENTARY NOTES Langley Technical Monitor: Dennis M. Bushnell Final Report Submitted to the Society of Experimental Mechanics (SEM) Conference Proceedings.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Unclassified Unlimited Subject Category 34 Distribution: Nonstandard Availability: NASA-CASI (301) 621-0390			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) Optimization of designs for nanotube-based scanning probes, which may be used for high-resolution characterization of nanostructured materials, is examined. Continuum models to analyze the nanotube deformations are proposed to help guide selection of the optimum probe. The limitations on the use of these models that must be accounted for before applying to any design problem are presented. These limitations stem from the underlying assumptions and the expected range of nanotube loading, end conditions, and geometry. Once the limitations are accounted for, the key model parameters along with the appropriate classification of nanotube structures may serve as a basis for the design optimization of nanotube-based probe tips.				
14. SUBJECT TERMS carbon nanotubes, atomic force microscope, scanning probes, optimization			15. NUMBER OF PAGES 10	
			16. PRICE CODE A03	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT	